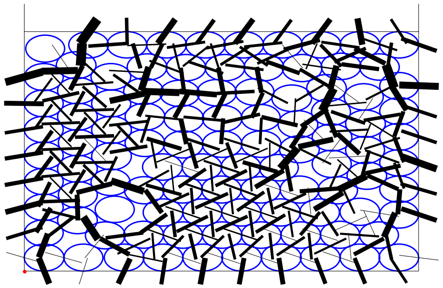
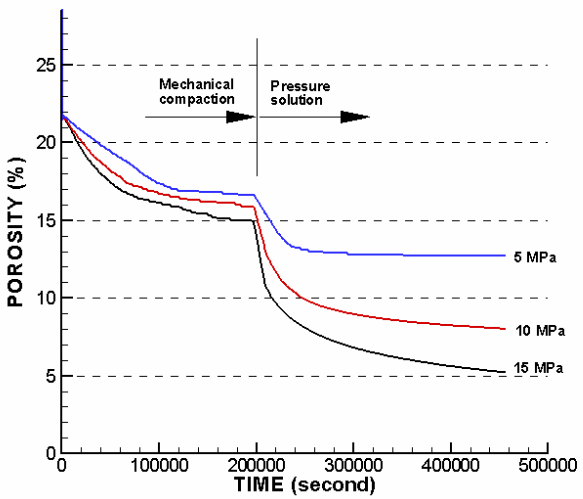
Distinct Element Modeling of Coupled Chemo-Mechanical Compaction of Rock Salt





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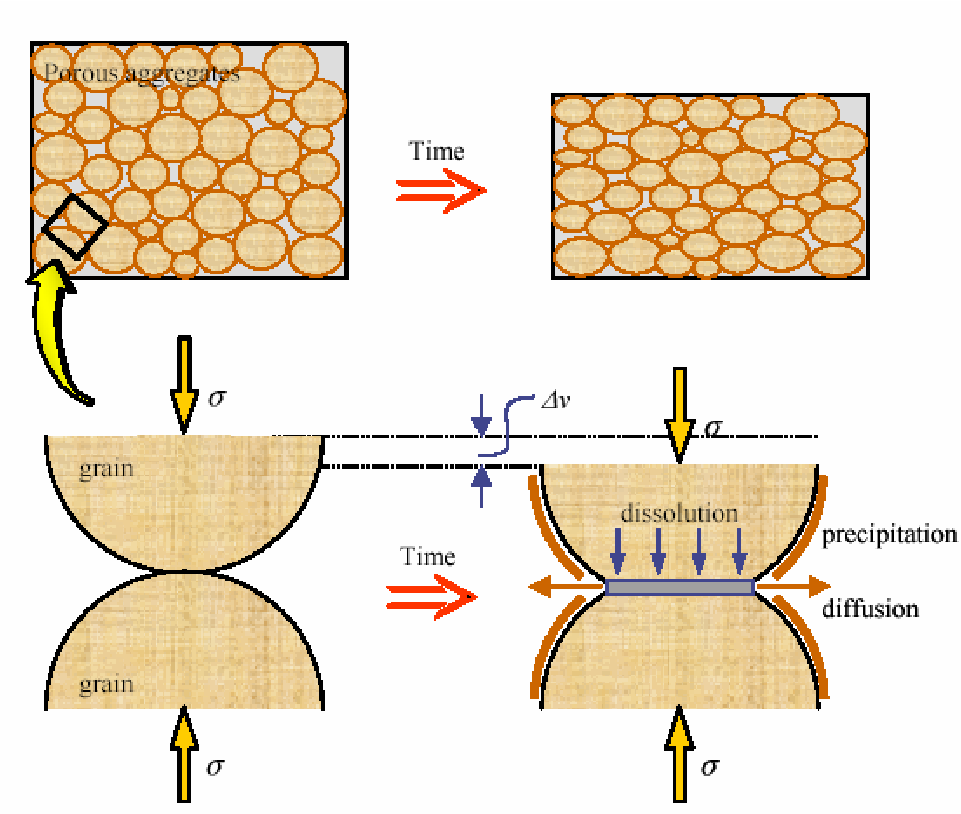
Outline

- Motivation
- Pressure solution process
- Distinct Element Method (DEM) and implementation of pressure solution
- Experimental results
- Numerical simulation
- Conclusion

Motivation

- Long-term rheological properties of rock salt are important – nuclear waste repository, salt mine, …
- Challenges in understanding chemical compaction
  - Conceptual model on compacted particles (models often on a single particle-particle contact)
  - Extrapolation necessary (very long term laboratory experiment not feasible)
- Numerical modeling can yield further understanding of the mechanism of chemical compaction

Pressure solution processes



Yasuhara et al., 2003, JGR

Three linked processes: dissolution, diffusion and precipitation

Three linked processes

- Interface Dissolution

$$\frac{dM_{diss}}{dt} \approx \dot{\varepsilon}_{diss} \frac{d}{\omega} \rho_g \left(\frac{\pi}{4} d_c^2 \omega \right)$$

$$= \frac{3\pi V_m^2 \sigma_{eff}\, k_+ \rho_g\, d_c^2}{4RT}$$

$$\frac{dM_{diss}}{dt} = \frac{3\pi V_m^2 (\sigma_a - \sigma_c) k_+ \rho_g\, d_c^2}{4RT}$$

$$\sigma_c = \frac{E_m \left(1 - T/T_m \right)}{4V_m}$$

- Interface Diffusion

$$J = -D_b \frac{dC}{dx} \qquad J_m = -2\pi r \varpi D_b \left(\frac{dC}{dr} \right)_{r=d_c}$$

$$J_m = \frac{dM_{diff}}{dt} = \frac{2\pi\, \omega\, D_b}{\ln\left(d_c / 2a \right)} \left(C_{\text{int}} - C_{pore} \right)$$

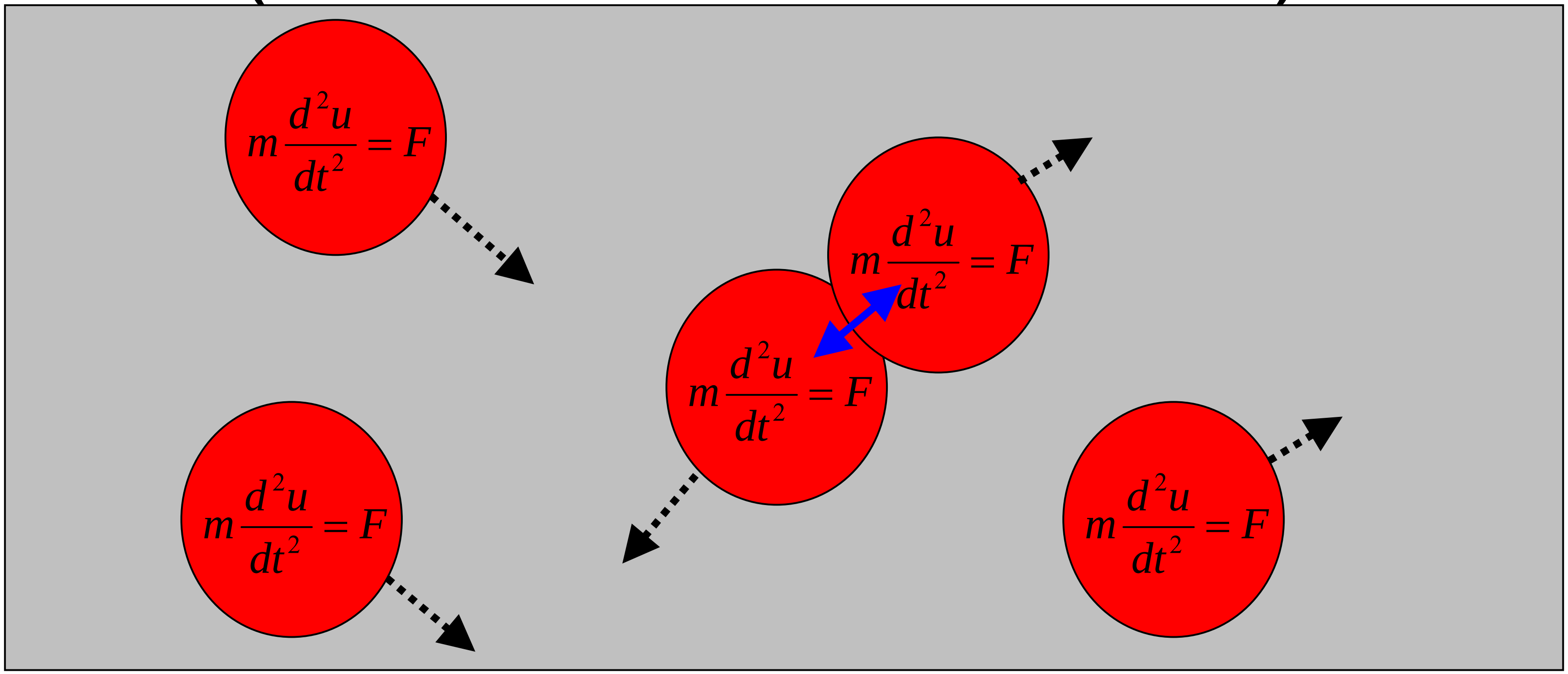
The slowest and rate controling process for rock salt!

- Pore Precipitation

$$\frac{dM_{prec}}{dt} = V_{pore} \frac{A}{M} k_- \left(C_{pore} - C_{eq} \right)$$

(Yasuhara et al., JGR, 2003)

Distinct(Discrete) Element Method (Cundall & Strack, 1979)



- Distinct Element Method (DEM) solves for motion of interacting particles by finite difference method.
- DEM recognizes new contacts within internal algorithm.
- Applications - powder mechanics, granular materials, also molecular dynamics (MD) simulations

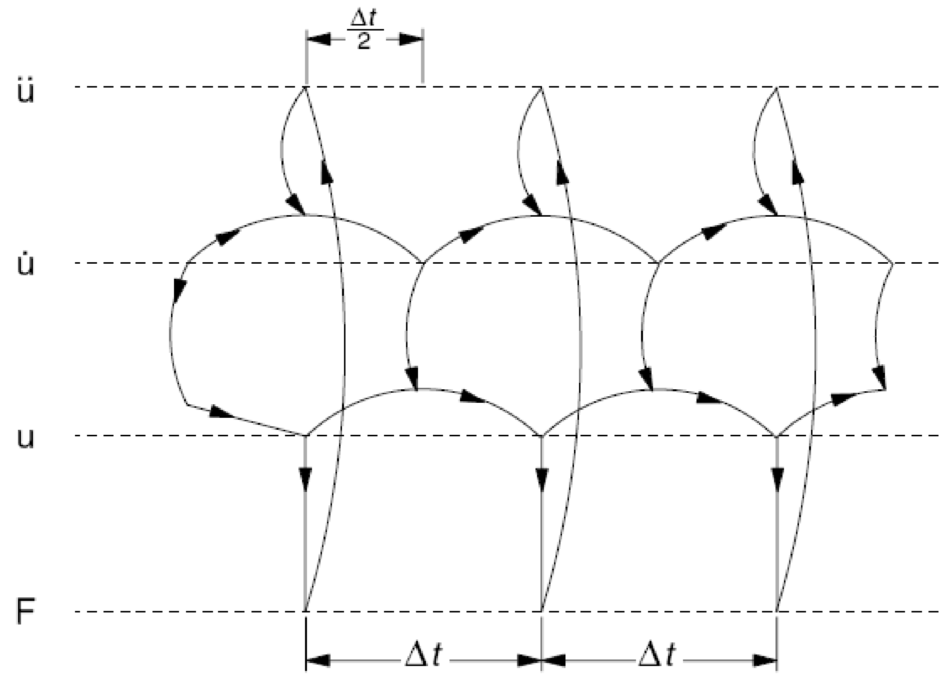
Time integration of equation of motion

- From central difference scheme

$$\dot{u}^{(t+\Delta t/2)} = \frac{u(t+\Delta t) - u(t)}{\Delta t}$$

$$\dot{u}^{(t+\Delta t/2)} = \dot{u}^{(t-\Delta t/2)} + \frac{F^{(t)}}{m}\Delta t$$

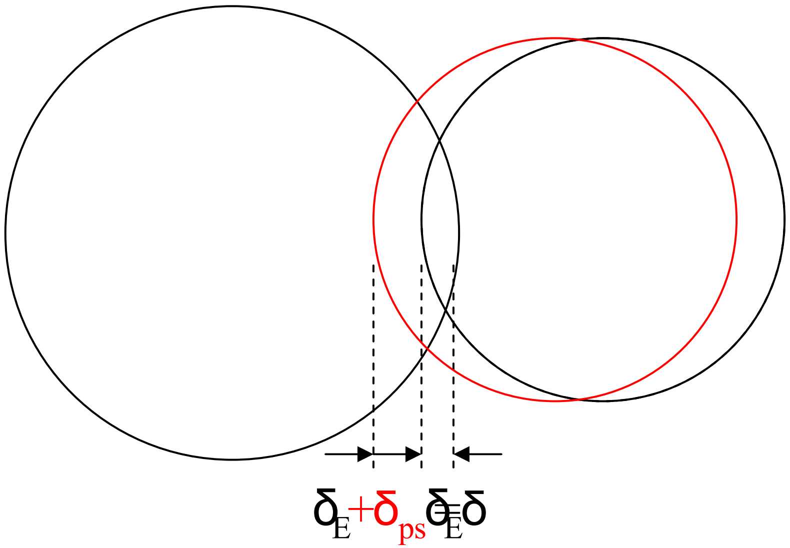
$$u^{(t+\Delta t)} = u^{(t)} + \dot{u}^{(t+\Delta t/2)}\Delta t$$



Itasca (2004)

The original paper by Cundall and Strack (1979) in Geotechnique on DEM attracted more than 1,300 citations! – unusually large number as a engineering paper. Most popular code is PFC by Itasca.

Contact displacement by pressure solution



$$\dot{\varepsilon}_{diff} = \frac{2\pi w D_b}{\ln(d_c / 2a)} \frac{(\sigma_a - \sigma_c)}{RT} V_m C_0 \frac{1}{\rho_d} \frac{1}{\left(\frac{\pi}{4}\right) d_c^{\,2}} \frac{1}{d}$$

$$\delta_{ps} = \dot{\varepsilon}_{diff} \cdot d \cdot dt$$

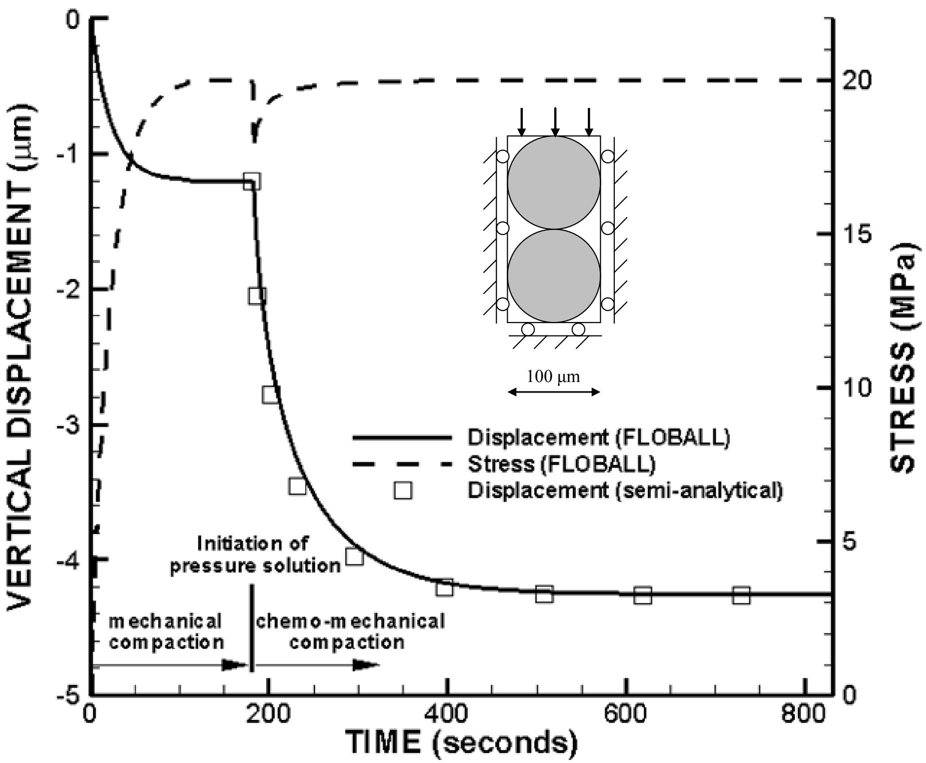
$$F = K \cdot \left(\delta - \delta_{ps}\right)$$

Implemented in serial connection

Diffusion is the slowest and rate limiting process

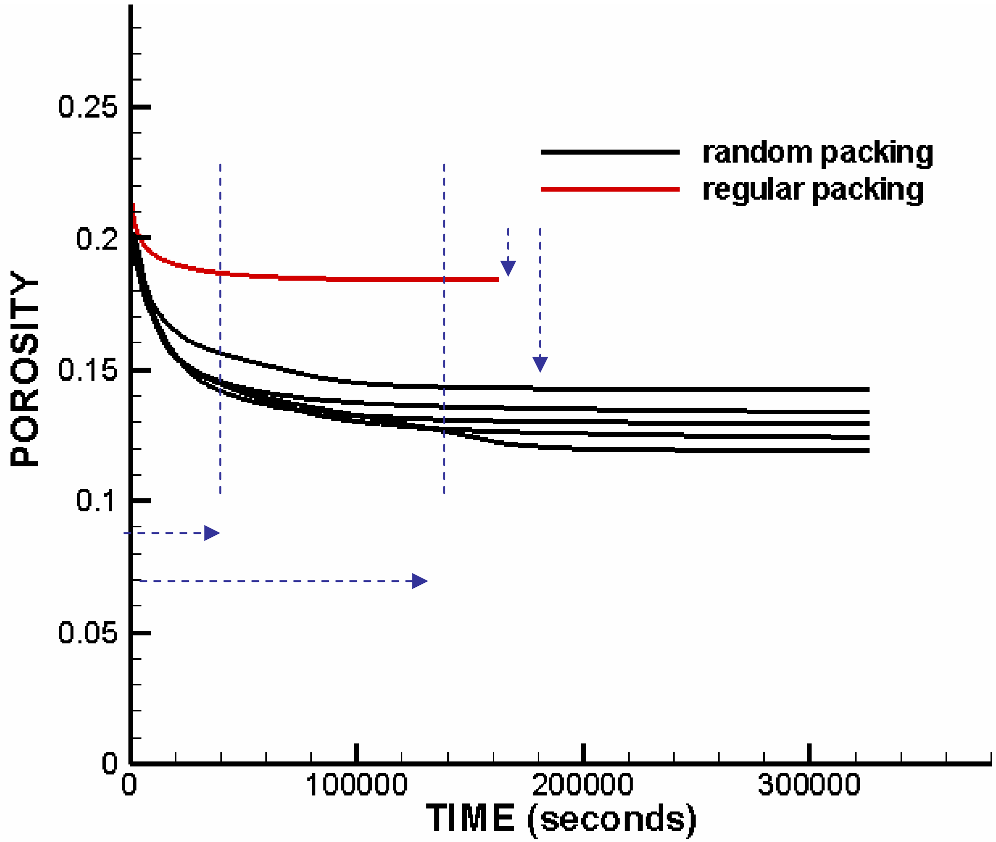
Pressure solution continues until it reaches a critical stress at the contact

Verification

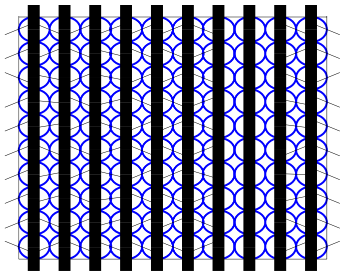


- Numerical experiment under servo controlled stress application.
- Implemented scheme gives satisfactory match between numerical and semi-analytical models for a two-particle system

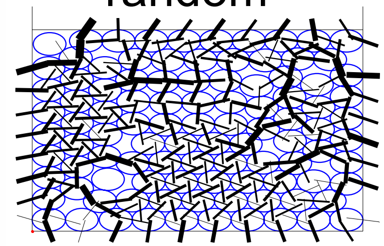
Regular compaction vs. random compaction



regular



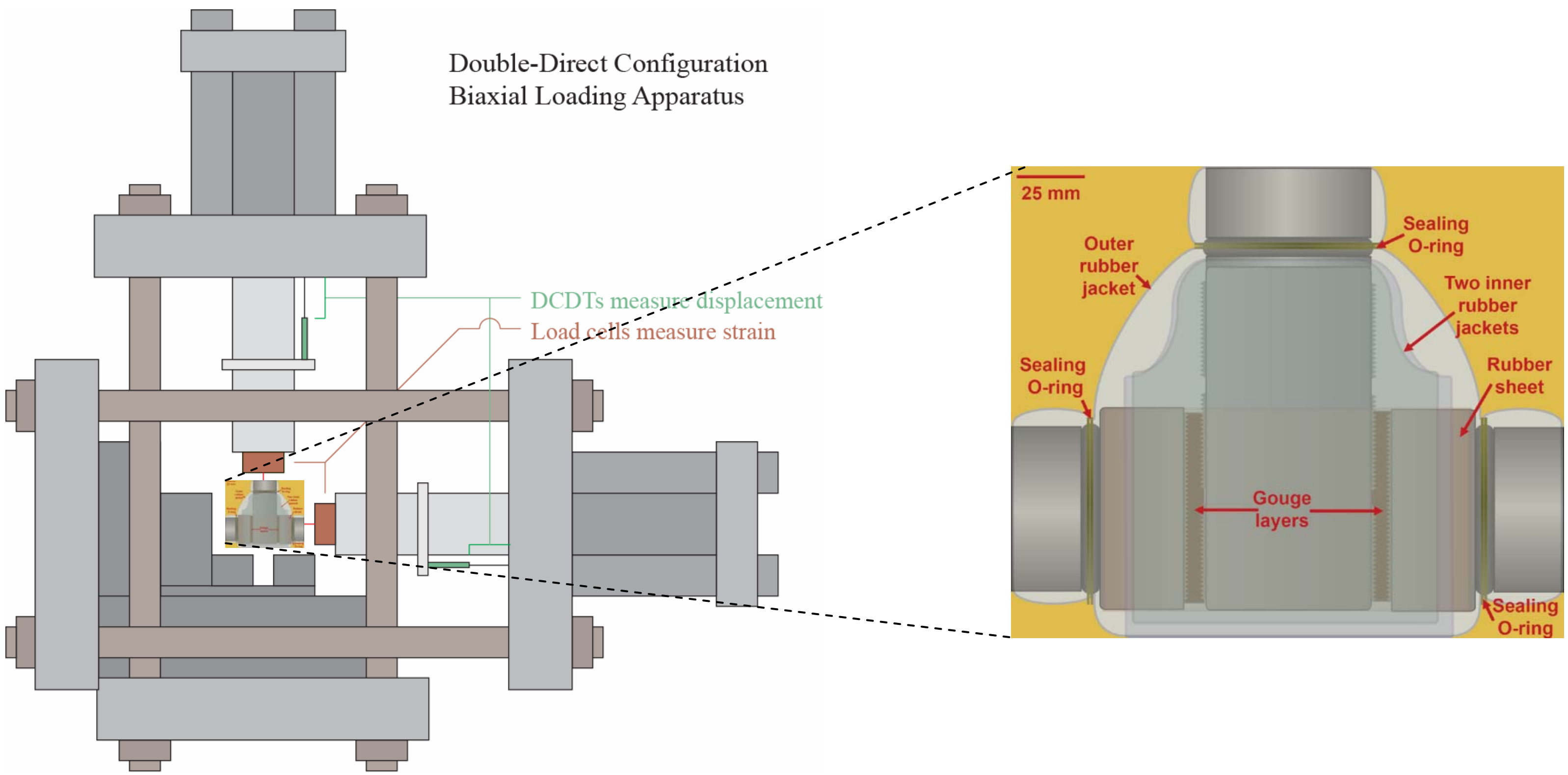
random



Force Distribution

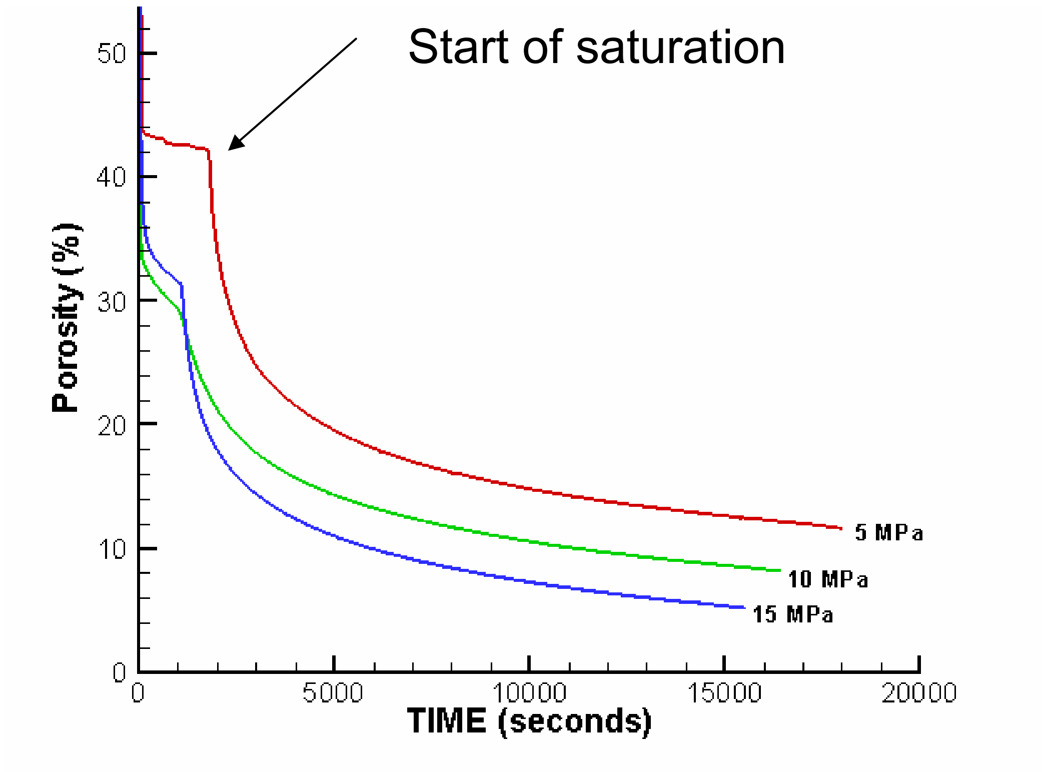
- Regular compaction model significantly underestimates the actual compaction anticipated in a randomly packed material – both magnitude and time

Laboratory experiment



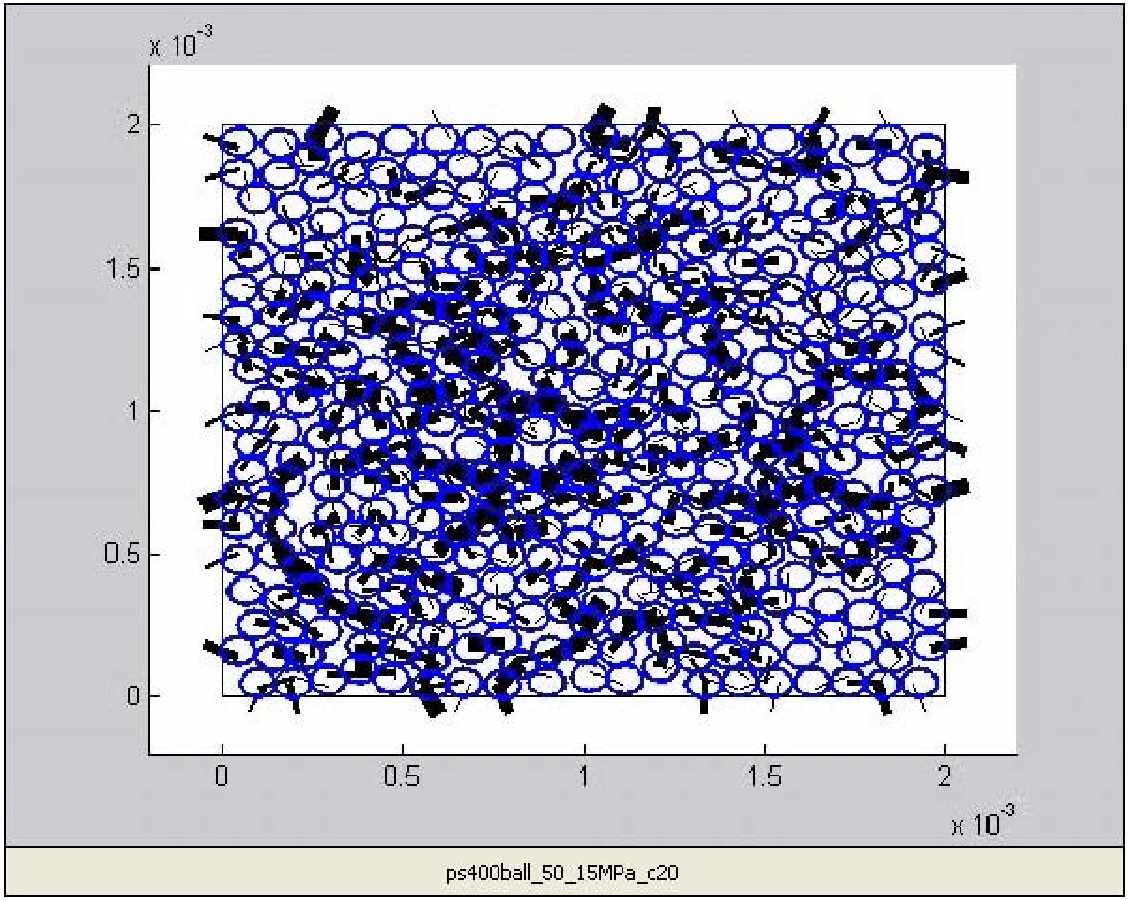
- Normal stress: 5, 10, 15 MPa, Pore pressure : 1 MPa
- Servo-controlled stresses with simultaneous measurement displacement (ref. Marone et al., this volume, p.17)
- Rock salt samples in a range of diameter distributions (e.g., 37-106 μm)

Experimental data



- Larger porosity reduction with increased normal stress, ~ 5 hours

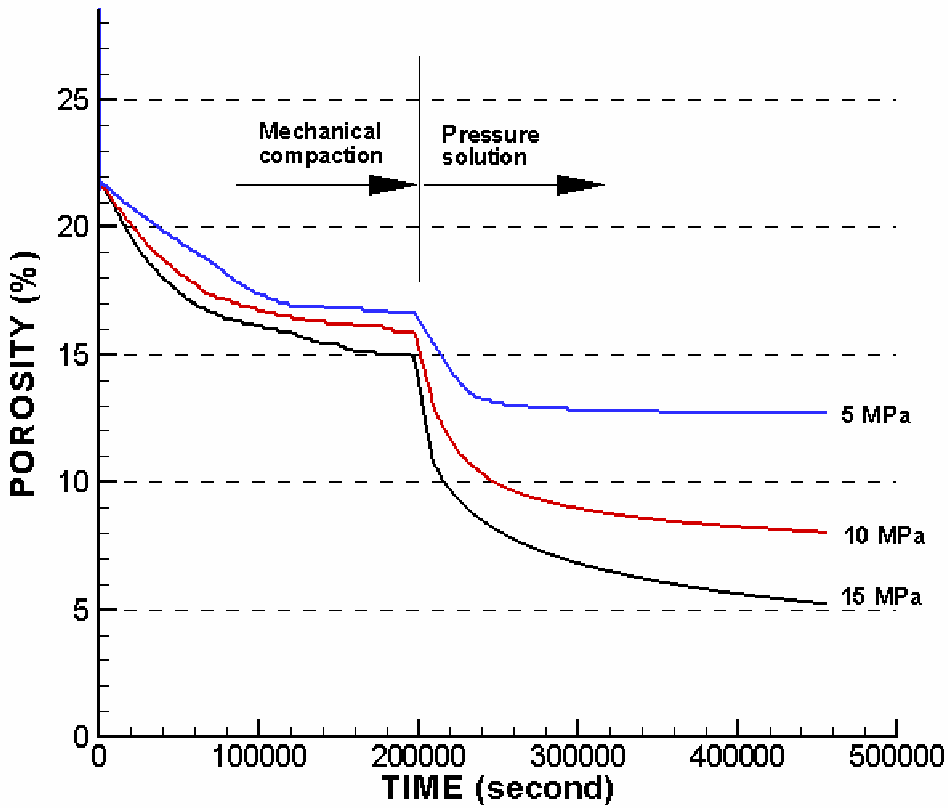
DEM modeling of compaction of rock salt



Loads are maintained same level through servo-control at the platen.

Mechanical compaction and chemical compaction during 3 days.

Porosity reduction from DEM modeling



Dissolution rate constant

= 2.51e-3 mol/m^2/s

Diffusion coefficient

= 1e-10 m^2/s

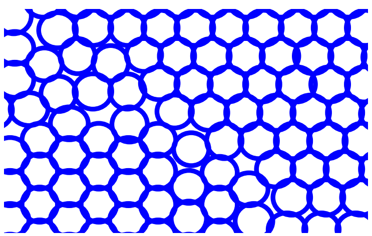
Diffusion path width = 100e-9 m

Solubility = 350 kg/m^3

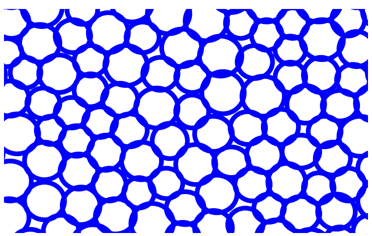
Critical stress = 20 MPa

- General trend is similar to experimental results, ~3 days
- Initial porosity much smaller than experiments – 2D vs 3D

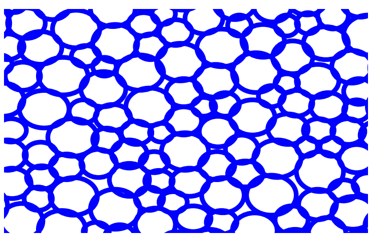
Comparison of constant vs. variable diameter of particles



D = 100 μm



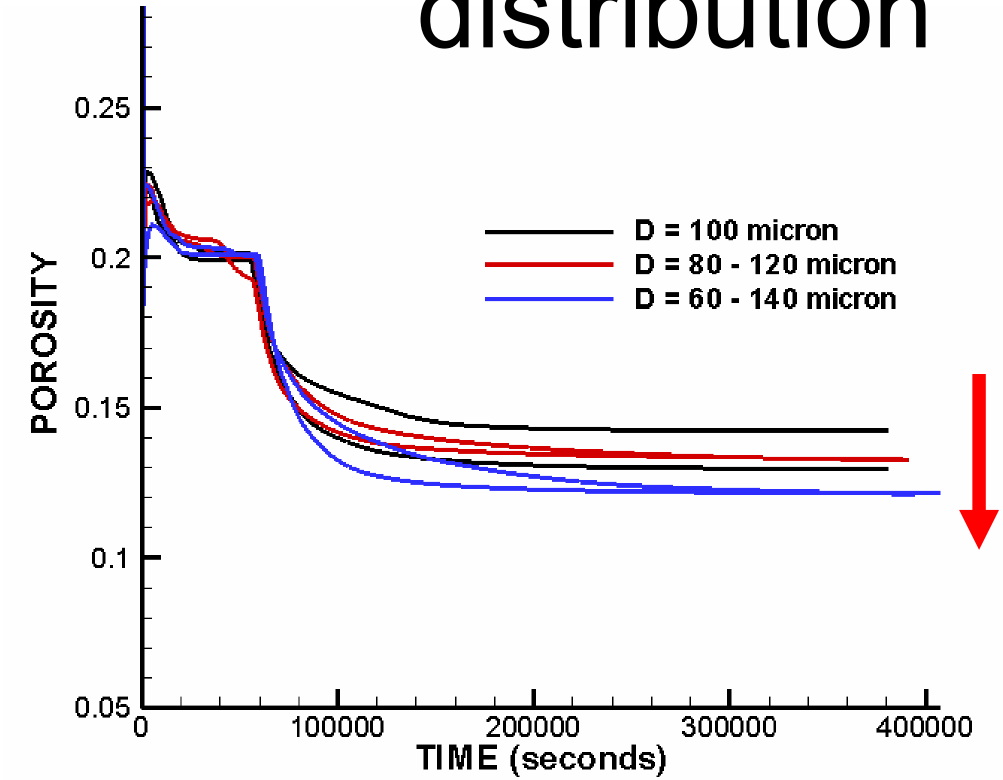
D = 80 - 120 μm
(uniform distr.)



D = 60 – 140 μm
(uniform distr.)

- Above distributions are tested to see the effect of diameter distribution – power of DEM
- Will distributed particle diameter increase the chemical compaction???

Compaction with different diameter distribution



Reduction of

Porosity

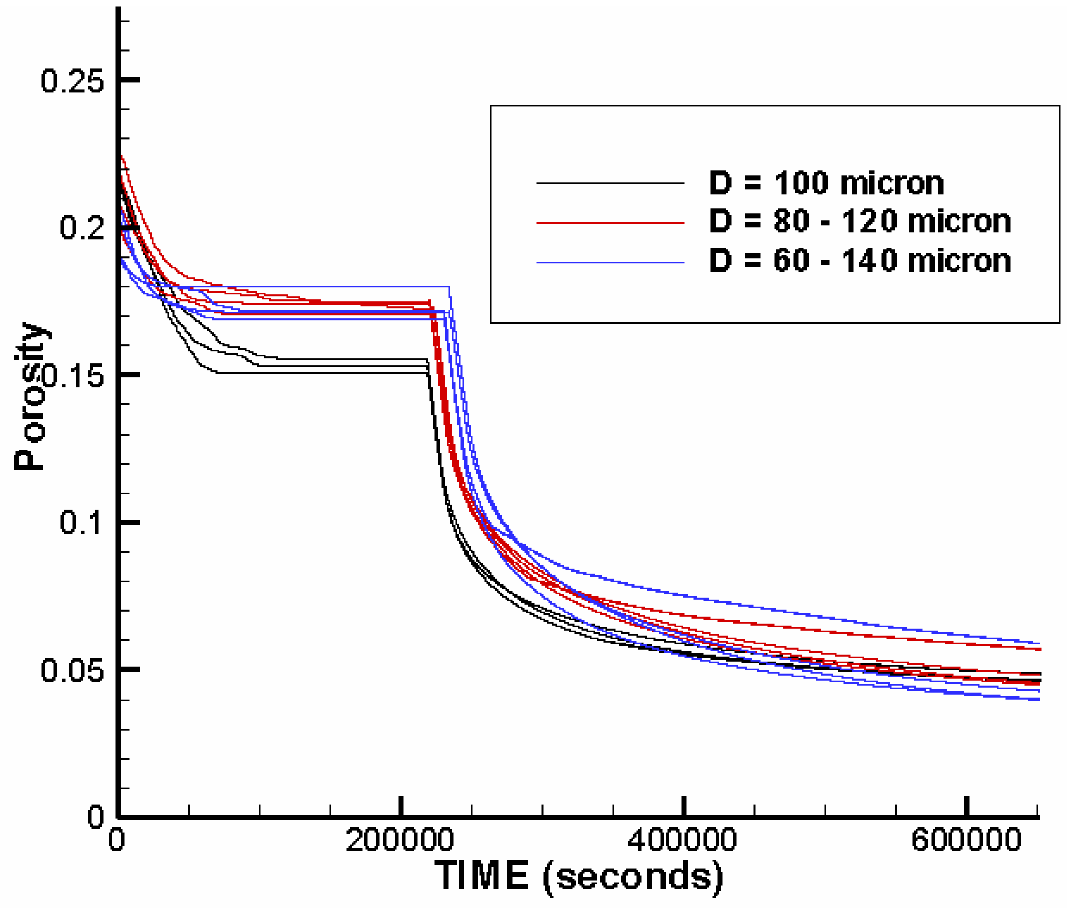
– not yet clear

- Models with more variable diameters seems to have more reduction of porosity - the magnitude is not substantial. Further investigation is needed.
- Needs to consider – number of contacts in each particles, actual initial porosity, additional experiment to see the effect of size distribution

Conclusion

- DEM modeling is an effective tool for the prediction of porosity(Φ) reduction – 1-D semi-analytical model may underestimate Φ
- DEM modeling captures the main features of compaction history
- Larger range of distribution seem to induce slightly more porosity reduction. However, the mechanism for this merits further investigation

- 3-D extension & inclusion of fluid flow in DEM code – future work



D = 100 micron
D = 80 - 120 micron
D = 60 - 140 micron
Porosity
0.25
0.2
0.15
0.1
0.05
0
0
200000
400000
600000
TIME (seconds)